Effective classical partition functions

R. P. Feynman
Lauritsen Laboratory, California Institute of Technology, Pasadena, California 91125

H. Kleinert*
Department of Physics, University of California, San Diego, La Jolla, California 92093
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We present a method by which a quantum-mechanical partition function can be approximated from below by an effective classical partition function. The associated potential is obtained by a simple smearing procedure. For a strongly anharmonic oscillator and a double-well potential, the lowest approximation gives a free energy which is accurate to a few percent, even at zero temperature.

The path-integral representation of a quantum-mechanical partition function[1]

$$Z\equiv e^{-\beta F}$$

$$\equiv \int \mathscr{D}x(\tau)\exp\left[-\int_0^\beta d\tau\left[\frac{\dot{x}^2(\tau)}{2}+V(x(\tau))\right]\right] \quad (1)$$

involves an infinite product of ordinary integrals which, after a Fourier decomposition of the periodic paths $x(\tau)=x_0+\sum_{n=1}^{\infty}(x_n e^{i\omega_n\tau}+\text{c.c.})$ with $\omega_n=2\pi n/\beta$ can be written as follows:[1]

$$Z=\int\frac{dx_0}{\sqrt{2\pi\beta}}\left[\prod_{n=1}^{\infty}\int\frac{dx_n^{\text{real}}\,dx_n^{\text{im}}}{\pi/(\beta\omega_n^2)}\times\exp\left[-\beta\sum_{n=1}^{\infty}\omega_n^2|x_n|^2-\int_0^\beta d\tau\,V(x(\tau))\right]\right]. \quad (2)$$

The x_n appear implicitly in $x(\tau)$, the argument of V. If we were able to perform the $n\neq 0$ integrals, this would leave Z as a simple integral

$$Z=\int\frac{dx_0}{\sqrt{2\pi\beta}}e^{-\beta W(x_0)}. \quad (3)$$

In the high-temperature limit we are able to do so. The kinetic terms $\omega_n^2|x_n|^2$, $n\neq 0$, develop very sharp minima around zero. The x_n are always small [of order $1/(\omega_n\sqrt{\beta})$] and may be neglected in $V(x(\tau))$. The integrals over $dx_n^{\text{real}}dx_n^{\text{im}}$ become trivial, resulting in the well-known classical limit $W(x)\to V(x_0)$ as $T\to\infty$:

$$Z\to Z_{\text{cl}}=\int\frac{dx_0}{\sqrt{2\pi\beta}}\exp\{-\beta V(x_0)\}.$$

Because of the similarity between this and (3) we shall refer to the function $W(x_0)$ as the effective classical potential[2] and to the integral (3) as the effective classical partition function.

At first sight, introducing $W(x_0)$ may seem of little use since the integrals over all x_n, $n\neq 0$, collected in $W(x_0)$ are, in general, impossible to perform. The purpose of this paper, however, is to show that for smooth potentials, $V(x)$, there exists a simple way of evaluating these integrals *approximately* to a very high accuracy, leading to an upper bound for $W(x_0)$, to be denoted by $W_1(x_0)$, and to be found according to the following rules.

(1) Calculate a smeared version of the potential $V(x)$ as follows:

$$V_{a^2}(x)\equiv\int\frac{dx'}{(2\pi a^2)^{1/2}}\exp\left[-\frac{1}{2a^2}(x-x')^2\right]V(x') \quad (4)$$

with an as yet unknown width parameter a^2.

(2) Introduce a second parameter Ω and form the auxiliary potential

$$\tilde{W}_1(x_0,a^2,\Omega)=\frac{1}{\beta}\ln\frac{\sinh(\beta\Omega/2)}{\beta\Omega/2}-\frac{\Omega^2}{2}a^2+V_{a^2}(x_0). \quad (5)$$

(3) Consider a^2,Ω as functions of x_0 and calculate, at each x_0, the minimum of $\tilde{W}_1(x_0,a^2(x_0),\Omega(x_0))$ with respect to the parameters $a^2(x_0)$ and $\Omega(x_0)$. The result is the desired approximate effective classical potential

$$W_1(x_0)=\min_{a^2(x_0),\Omega(x_0)}\{\tilde{W}_1(x_0,a^2(x_0),\Omega(x_0))\}. \quad (6)$$

Explicitly, the minimization with respect to Ω gives, at each x_0, the following relation between Ω and a^2:

$$a^2=\frac{1}{\beta\Omega^2}\left[\frac{\beta\Omega}{2}\coth\left[\frac{\beta\Omega}{2}\right]-1\right], \quad (7)$$

while the minimization in a^2 determines Ω^2 as a function of the smeared potential:

$$\Omega^2(x_0)=2\frac{\partial}{\partial a^2}V_{a^2}(x_0)=\frac{\partial^2}{\partial x_0^2}V_{a^2}(x_0)\,. \tag{8}$$

The derivation of these rules starts out with a trial partition function Z_1 in which the effect of the potential energy upon the $n\neq 0$ components x_n is approximated by a Gaussian potential as follows:

$$Z_1\equiv e^{-\beta F_1}=\int \mathscr{D}x(\tau)\exp\left[-\int_0^\beta d\tau\left[\frac{\dot{x}^2(\tau)}{2}+\frac{\Omega^2(x_0)}{2}[x(\tau)-x_0]^2\right]-\beta L_1(x_0)\right], \tag{9}$$

where $\Omega^2(x_0)$ is an arbitrary local curvature of the potential and $L_1(x_0)$ is a trial potential depending only on the average coordinate x_0. Both functions $\Omega(x_0)$ and $L_1(x_0)$ will be determined by an extremal principle.

The ansatz (9) has the virtue that all x_n with $n\neq 0$ can be integrated out leaving only an integral over x_0

$$Z_1=\int\frac{dx_0}{\sqrt{2\pi\beta}}\frac{\beta\Omega(x_0)/2}{\sinh[\beta\Omega(x_0)/2]}e^{-\beta L_1(x_0)}\,. \tag{10}$$

Moreover, it is straightforward to calculate, within the trial partition function Z_1, the expectation of the difference between the true and the trial potential

$$\left\langle\left[V(x(\tau))-\frac{\Omega^2(x_0)}{2}[x(\tau)-x_0]^2\right]-L_1(x_0)\right\rangle_1, \tag{11}$$

where

$$\langle O\rangle_1\equiv Z_1^{-1}\int\mathscr{D}x(\tau)O\exp\left[-\int_0^\beta d\tau\left[\frac{\dot{x}^2(\tau)}{2}+\frac{\Omega^2(x_0)}{2}[x(\tau)-x_0]^2\right]-\beta L_1(x_0)\right]. \tag{12}$$

Indeed, if we use the Fourier representation of the paths and for $V(x(\tau))$ a Fourier representation in space, writing

$$V(x(\tau))=\int\frac{dq}{2\pi}\tilde{V}(q)\exp\left\{iq\left[x_0+\left[\sum_{n=1}^\infty x_n e^{i\omega_n\tau}+\text{c.c.}\right]\right]\right\}, \tag{13}$$

the expectation of $V(x(\tau))$ can be brought to the form

$$\langle V(x(\tau))\rangle_1=Z_1^{-1}\int\frac{dx_0}{\sqrt{2\pi\beta}}\prod_{n=1}^\infty\int\frac{dx_n^{\text{real}}dx_n^{\text{im}}}{\pi/(\beta\omega_n^2)}\int\frac{dq}{2\pi}\tilde{V}(q)\exp\left\{-\beta\sum_{n=1}^\infty[\omega_n^2+\Omega^2(x_0)]\,|x_n|^2-\beta L_1(x_0)+iq\left[x_0+\left[\sum_{n=1}^\infty x_n e^{i\omega_n\tau}+\text{c.c.}\right]\right]\right\} \tag{14}$$

in which all x_n, $n\neq 0$, can again be integrated out. The result is

$$\langle V(x(\tau))\rangle_1=Z_1^{-1}\int\frac{dx_0}{\sqrt{2\pi\beta}}\frac{\beta\Omega(x_0)/2}{\sinh[\beta\Omega(x_0)/2]}e^{-\beta L_1(x_0)}V_{a^2(x_0)}(x_0)\,, \tag{15}$$

where $V_{a^2(x_0)}(x_0)$ is the smeared potential (4) with

$$a^2(x_0)\equiv\frac{2}{\beta}\sum_{n=1}^\infty\frac{1}{\omega_n^2+\Omega^2(x_0)}\,. \tag{16}$$

This can be summed up to give the expression (7).

The Gaussian potential $\frac{1}{2}\Omega^2(x_0)[x(\tau)-x_0]^2$ can be considered as a particular case of $V(x(\tau))$ and its smeared version $V_{a^2(x_0)}(x_0)$ becomes simply $\frac{1}{2}\Omega^2(x_0)a^2(x_0)$. Hence, the expectation (11) reads

$$Z_1^{-1}\int\frac{dx_0}{\sqrt{2\pi\beta}}\frac{\beta\Omega(x_0)/2}{\sinh[\beta\Omega(x_0)/2]}e^{-\beta L_1(x_0)}\times\left[V_{a^2(x_0)}(x_0)-\frac{\Omega^2(x_0)}{2}a^2(x_0)-L_1(x_0)\right]. \tag{17}$$

The unknown functions $\Omega^2(x_0), L_1(x_0)$, are now determined by using the extremal principle explained in Ref. 1, Sec. 10.3. It is based on the well-known inequality for convex functionals which states that the true partition function Z is bounded from below by

$$Z > Z_1 \exp\left[-\left\langle \int_0^\beta d\tau \left[V(x(\tau)) - \frac{\Omega^2(x_0)}{2}[x(\tau)-x_0]^2 - L_1(x_0)\right]\right\rangle_1\right]. \quad (18)$$

Using (10) and (17) and performing the variations in $\Omega(x_0)$ and $L_1(x_0)$ we see that the best lower bound is obtained when the integrand of (17) vanishes *identically* in x_0. This fixes

$$L_1(x_0) = V_{a^2(x_0)}(x_0) - \frac{\Omega^2(x_0)}{2} a^2(x_0) .$$

Equation (10) has the form (3) with $W(x_0)$ being bounded from above locally by $\tilde{W}_1$ of Eq. (5). The bound is further improved by minimizing $\tilde{W}_1$ with respect to $\Omega(x_0)$ which yields $W_1(x_0)$ and thus the result stated in the beginning.

As an example, let us apply the procedure to the anharmonic oscillator with $V(x)=\frac{1}{2}x^2+\frac{1}{4}gx^4$. The smeared potential (4) is

$$V_{a^2} = \tfrac{1}{2}a^2 + \tfrac{3}{4}ga^4 + \tfrac{1}{2}(1+3ga^2)x^2 + \tfrac{1}{4}gx^4 ,$$

from which we find, via (8), $\Omega^2 = 1+3ga^2+3gx^2$. We now solve Eqs. (7) and (8) at each x_0 by iteration, and calculate $W_1(x_0)$ from Eqs. (5) and (6). The free energies F_1 resulting from the integral (3) are shown in Fig. 1 and compared with the exact F_{ex}, the classical F_{cl}, and an earlier upper bound F_0, derived via the method of Ref. 1, Sec. 10.3, which corresponds to the special nonminimal choice for Ω, $\Omega \equiv 0$, so Eq. (7) gives $a^2=\beta/12$.

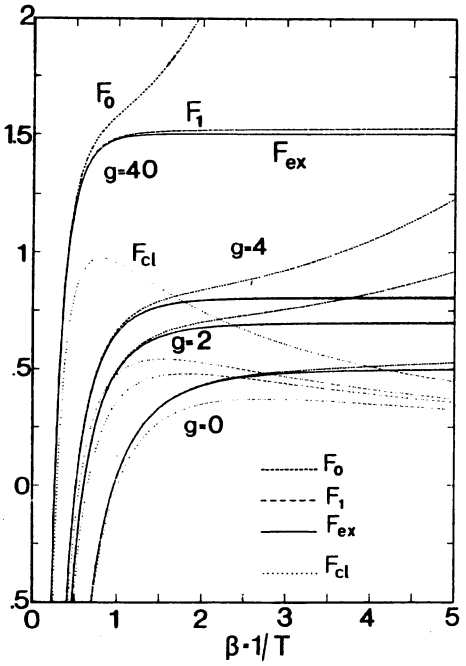

FIG. 1. Different approximate free energies F_1 (ours); F_0 (earlier Feynmann's), F_{cl} (classical); compared with F_{ex} (exact), for the anharmonic oscillator potential $V(x)=\frac{1}{2}x^2+\frac{1}{4}gx^4$, as a function of $\beta \equiv 1/T$, with anharmonic couplings $g=0,2,4,40$. Notice that F_{cl} lies far below the exact curve, while F_0 lies far above it. The new F_1, on the other hand, fits extremely well, up to a few percent, for all g and down to zero temperature. For $g \lesssim 4$, the difference between F_1 and F_{ex} is hardly visible.

Even for strong anharmonicity ($g=40$), the result is good down to $T=0$, up to 3% accuracy. The high quality of the approximation can be understood by observing that, in general, the $T \to 0$ limit of F_1 is

$$F_1 \underset{T\to 0}{\to} E^0 \equiv \min_{T=0}\{W_1(x_0)\} = \min_{a^2}\{V_{a^2} + 1/8a^2\} \quad (19)$$

which is the same as the minimal expectation value of the Schrödinger operator $\hat{H} = -\frac{1}{2}\partial^2 + V(x)$ in a Gaussian wave packet $(2\pi a^2)^{-1/4}\exp(4a^2x^2)$. For the anharmonic oscillator, the minimum is reached at $a^2=[2(1+3ga^2)^{1/2}]^{-1}$. A Gaussian wave packet is known to give extremely good ground-state energies for many smooth symmetric potentials. Table I compares the energies obtained in this way with the known ground-state energies of the anharmonic oscillator[3] up to $g=4000$.

Another example is the double-well potential $V(x)=-\frac{1}{2}x^2+\frac{1}{4}x^4+1/4g$. When solving Eqs. (7) and (8), the quantity $\Omega^2(x_0)$ may become negative for $x_0 \approx 0$. This, however, presents no problem since there is always a solution $\Omega^2(x_0)$ which remains in the interval $\Omega^2 \in (-4\pi^2T^2, \infty)$ for which $a^2>0$ [see Eq. (16)]. The various free energies F_1 are shown in Fig. 2. They are in slightly worse agreement with the exact ones than those in Fig. 1, although our approximation is quite reliable up to $\beta \approx 5$. Notice that at $T=0$, the quantum fluctuations wipe out the double well for large $g \gtrsim 0.36$ (see Fig. 3). For $g \lesssim 0.36$, the two off-centered minima survive. They become lower than the central minimum for $g \lesssim 0.325$. In each case, the absolute minimum gives the position of the optimal Gaussian wave packet. Table II compares the energy E^0 with the true ground-state energies E^0_{ex} which shows that the worst possible ($T=0$) error of our approximation is $\lesssim 16\%$ for $g \approx 0.4$.

Our method can easily be extended to the n-dimensional Schrödinger problem in which $x_i=(\mathbf{x})_i$ is an n-component vector and trial frequency $[\Omega^2(\mathbf{x}_0)]_{ij}$ in (9) an $n\times n$ matrix. In the special case that $V(x_i)=V(\mathbf{x}^2)$ is rotationally symmetric, we may introduce longitudinal and transverse parts of Ω^2_{ij} via

$$\Omega^2_{ij} \equiv \Omega^2_L(\mathbf{x}_0^2)x_{0i}x_{0j}/\mathbf{x}_0^2 + \Omega^2_T(\mathbf{x}_0^2)(\delta_{ij} - x_{0i}x_{0j}/\mathbf{x}_0^2)$$

and W_1 becomes

$$\tilde{W}_1 = \frac{1}{\beta}\left[\ln\left[\frac{\sinh(\beta\Omega_L/2)}{\beta\Omega_L/2}\right] + (n-1)\ln\left[\frac{\sinh(\beta\Omega_T/2)}{\beta\Omega_T/2}\right]\right] - \tfrac{1}{2}[\Omega^2_L a^2_L + (n-1)\Omega^2_T a^2_T] + V_{a^2_L, a^2_T}(\mathbf{x}_0^2) , \quad (20)$$

where the smeared potential is

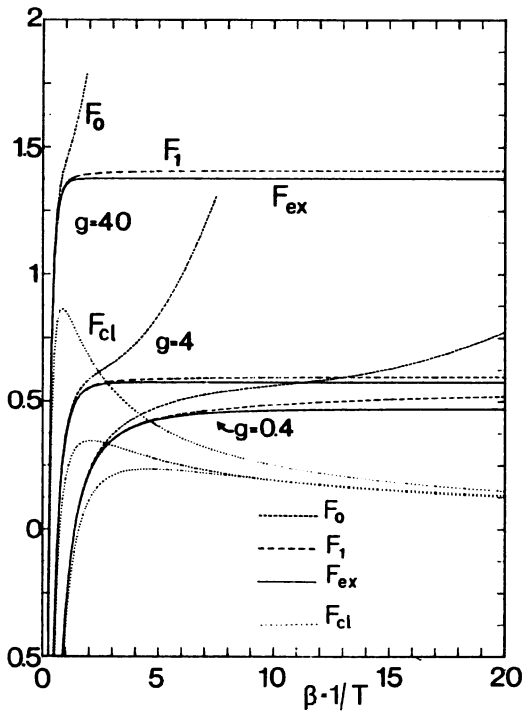

FIG. 2. Same plot as in Fig. 1, but for the double-well potential $V(x)=-\frac{1}{2}x^2+\frac{1}{4}gx^4+1/4g$.

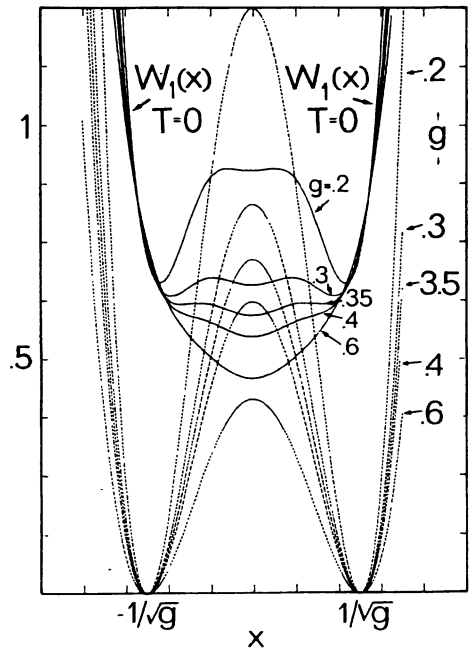

FIG. 3. Effective classical potential $W_1(x)$ at $T=0$ (——) and ∞ (- - -) [where $W_1(x)=V(x)$] for the double-well potential $V(x)=-\frac{1}{2}x^2+\frac{1}{4}gx^4+1/4g$ at various values of g.

$$V_{a_L^2,a_T^2}(\mathbf{x}^2)=\frac{1}{(2\pi a_L^2)^{1/2}}\frac{1}{(2\pi a_T^2)^{1/2(n-1)}}$$

$$\times\int d^nx'\exp\{-\tfrac{1}{2}(x'-x)_i[a_L^2x_ix_j/\mathbf{x}^2+a_T^2(\delta_{ij}-x_ix_j/\mathbf{x}^2)](x'-x)_j\}V(\mathbf{x}'^2)\,. \tag{21}$$

In principle, it is possible to generalize our method and treat also a few components x_n with $N\geq n>0$ more accurately. Using an Ansatz similar to (9), but with trial functions $\Omega^2(n_0,\ldots,x_N)$, $L_1(x_0,\ldots,x_N)$. The additional work, however, proliferates rapidly. The improvement proceeds from high to low T and the $T\to0$ limit is the same for any finite N.

Notice that the Ansatz (9) cannot be improved by allowing the trial function $\Omega^2(x_0)$ to be a matrix $\Omega^2_{nn'}(x_0)$ in the space of Fourier components x_n [i.e., by using $\sum_{n,n'}\Omega^2_{nn'}(x_0)x_n^\dagger x_{n'}$ instead of $\Omega^2(x_0)\sum_n|x_n|^2$] which would also lead to an exactly integrable trial partition function. After going through the minimization procedure, we would fall back upon our solution $\Omega^2_{nn'}(x_0)=\delta_{nn'}\Omega^2(x_0)$.

Let us further point out that by inserting an external source it is possible to calculate approximate correlation functions

$$\langle x(\tau)x(0)\rangle_1=\left\langle\left[x_0^2-\frac{1}{\beta\Omega^2(x_0)}\right]+G(\tau)\right\rangle_1,$$

where $G(\tau)$ is the periodic temperature Green's function which includes the zero-frequency part

TABLE I. Comparison of exact ground-state energy (Ref. 3) E^0_{ex} with the limit $E^0=\lim_{T\to0}F_1$ which is equal to the minimum of $W_1(x_0)$ at $T=0$ and can be obtained by minimizing the energy expectation of a Gaussian wave function centered at $x_0=0$. We also have listed the energy of the first two excited states E^1_{ex} and E^2_{ex}. Level splitting to the first excited state is given in column 6. We see that it is well approximated by the values of $\Omega(0)$ at $T=0$, as it should, due to Eq. (22).

g	E^0	E^0_{ex}	E^1_{ex}	E^2_{ex}	$E^1_{ex}-E^0_{ex}$	$\Omega(0)$	$a^2(0)$
2	0.7017	0.696 176	2.324 41	4.327 52	1.628 23	1.627	0.2991
4	0.8125	0.803 771	2.737 89	5.179 29	1.934 12	2.000	0.2500
40.0	1.5313	1.504 97	5.321 61	10.3471	3.816 94	4.000	0.1250
4000.0	6.8279	6.694 22	23.9722	47.0173	17.2780	18.190	0.0275

TABLE II. Same comparison as in Table I, but now for the double-well potential (Ref. 4). At small g, the minimum of the effective classical potential at $T=0$ lies at $x_0=\pm x_{\min}\neq 0$.

g	E^0	E^0_{ex}	E^1_{ex}	E^2_{ex}	$E^1_{ex}-E^0_{ex}$	$E^2_{ex}-E^0_{ex}$	$x_{\min}$	$\Omega(x_{\min})$	$a^2(x_{\min})$
0.1976	0.650	0.6192	0.6730	1.51	0.0538	0.891	1.943	1.255	0.397
0.4	0.549	0.4709	0.767 76	1.634 85	0.296 86	1.164	0	0.486	1.030
4.0	0.598	0.577 280 42	2.083 052 12	4.253 571 28	1.505 77	3.676	0	1.634	0.3059
40.0	1.409	1.377 816 85	4.995 666 52	9.894 742 35	3.617 85	8.517	0	3.829	0.1306

$$G(\tau)\equiv\frac{1}{\beta}\sum_{n=-\infty}^{\infty}e^{i\omega_n\tau}\frac{1}{\omega_n^2+\Omega^2}=\frac{1}{\beta\Omega^2}\frac{\sinh[(\beta-\tau)\Omega/2]}{\sinh(\beta\Omega/2)},$$

whose $\tau=0$ value is $a^2+1/\beta\Omega^2$. This can be continued analytically to the real time retarded Green's function

$$G^R(t)=\Theta(t)\langle x(t)x(0)\rangle_1$$
$$=-i\Theta(t)\left\langle\frac{1}{\Omega(x_0)}\sin(\Omega(x_0)t)\right\rangle_1 \tag{22}$$

showing that, for $T=0$, the quantity $\Omega(x_0)$ at the potential minimum $x_{\min}$ gives an approximation to the energy difference between ground and first excited state. In Table I we see that for the anharmonic oscillator this approximation is quite good. For the double-well potential, it is only good at large g. At small g, when the central barrier is very high, our approximation lacks the ability of describing tunneling. Therefore, $\Omega(x_{\min})$ at $T=0$ is not the small level splitting caused by tunneling but the distance between the lowest and the second *pair* of almost degenerate energy levels. (See Table II.)

Finally, let us remark that the method is useful also for some singular potentials as long as the smearing procedure makes sense. An example is the Yukawa potential $V(r)=-e^{-mr}/r$ where

$$V_{a^2}(\mathbf{x})=-\frac{2e^{m^2a^2/2}}{\sqrt{\pi}\,|\mathbf{x}|}\int_0^{|\mathbf{x}|/(2a^2)^{1/2}}dt\times\exp\left[-\left[t^2+\frac{m^2|\mathbf{x}|^2}{4t^2}\right]\right]$$

which in the Coulomb limit $m\to 0$ reduces to $-1/|\mathbf{x}|$ times the error function $\mathrm{erf}[|\mathbf{x}|/(2a^2)^{1/2}]$. In the latter case, the limit (19) becomes

$$E^0=\min_{a^2}\left\{\frac{3}{8a^2}+V_{a^2}(0)\right\}$$
$$=\min_{a^2}\left\{\frac{3}{8a^2}-\frac{2}{\sqrt{\pi}}\frac{1}{(2a^2)^{1/2}}\right\}.$$

The minimum is reached at $a^2_{\min}=9\pi/32$ and gives $E^0=-4/3\pi$. This is only 15% different from the true ground-state energy $-\frac{1}{2}$ such that, after subtracting the continuum contribution, the effective classical free energy F_1 of a Yukawa potential obtained by our method is, at any temperature, more accurate than this.

We do not want to end without mentioning a number of papers[5] which all have added improvements to our first attempts[1] at calculating an effective classical potential. It appears to us that our approximation $W_1(x_0)$ is both more accurate and easier to handle than any of its predecessors [we were able to use a simple home computer for doing the iteration of Eqs. (7) and (8) and the numeric integration (3)]. It will be interesting to extend the method to quantum field theories and to models of statistical mechanics.[6]

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*On sabbatical leave from the Institute for Theoretical Physics, Free University of Berlin, Arnimallee 14, D-1000 Berlin 33, Federal Republic of Germany.

[1]See, R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[2]Our "effective classical potential" must not be confused with the conventional "effective potential" of quantum field theory $V_{\text{eff}}(X)$. That is defined via the Legendre transform of the generating functional $W[j]$ of connected Green's functions. See, C. De Dominicis, J. Math. Phys. 3, 983 (1962); C. De Dominicis and P. C. Martin, *ibid.* 5, 16, 31 (1964); H. Dahmen and G. Jona-Lasino, Nuovo Cimento 52A, 807 (1967); A. N. Vasilev and A. K. Kazinskii, Theor. Math. Phys. 12, 875 (1972); J. M. Cornwall, R. Jackiw, and E. Tomboulis, Phys. Rev. 10, 2428 (1974); and the recent review by H. Kleinert, Fortschr. Phys. 30, 187 (1982). The relation between the two is that, for constant j, $e^{W[J]}$ is the Fourier transform of $e^{-\beta W(x_0)}$. It is an important virtue of our approach that even the lowest approximation to $W(x_0)$, in which one sets $W(x_0)=V(x_0)$, leads to a $V_{\text{eff}}(X)$ which is convex, a property of $V_{\text{eff}}(X)$ which by other approximation procedures is usually hard to achieve; see, for instance, Y. Fujimoto, L. O'Raifeartaigh, and G. Parravicini, Nucl. Phys. B212, 268 (1983).

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